Access DB# 1 ~ U 1 1

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Melanie Bissett Examiner # : 77899 Date: 2/1/05
Art Unit: 1711 Phone Number 30 571-272-1068 Serial Number: 10/629016
Mail Box and Bldg/Room Location: Rem 10D78 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: See attached

Inventors (please provide full names): Masaaki Tani, Yoshiaki Fukushima, Toshihisa Shimo

Earliest Priority Filing Date: 8/5/02 foreign filing

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

See attached claim for a mixture of Ti alkoxide w/ 2- or 3-layered compound of tetrahedral and octahedral layers. See also attached drawing of layer structure.

****

STAFF USE ONLY		Type of Search		Vendors and cost where applicable	
Searcher:	EL	NA Sequence (#)		STN	$ 363.53
Searcher Phone #:		AA Sequence (#)		Dialog	
Searcher Location:		Structure (#)	✓ (1)	Questel/Orbit	
Date Searcher Picked Up:		Bibliographic	✓ (and)	Dr.Link	
Date Completed:	2-3-05	Litigation		Lexis/Nexis	
Searcher Prep & Review Time:	5	Fulltext		Sequence Systems	
~~Clerical Prep Time:~~		Patent Family		WWW/Internet	
Online Time:	100	Other		Other (specify)	

What is claimed is:

1. A paint composition, comprising:

a layer organic-inorganic composite; and

titanium alkoxide in an amount of from 1 to 50 parts by weight with respect to the layer organic-inorganic composite taken as 100 parts by weight;

the layer organic-inorganic composite composed of a laminated substance comprising:

a tetrahedral structural layer made of tetrahedral structures whose central atom M′ is Si or a first metallic atom substituting for a part the Si, at least a part of the central atom M′ covalent-bonded to an organic group R involving or free from a polymerizable functional group; and

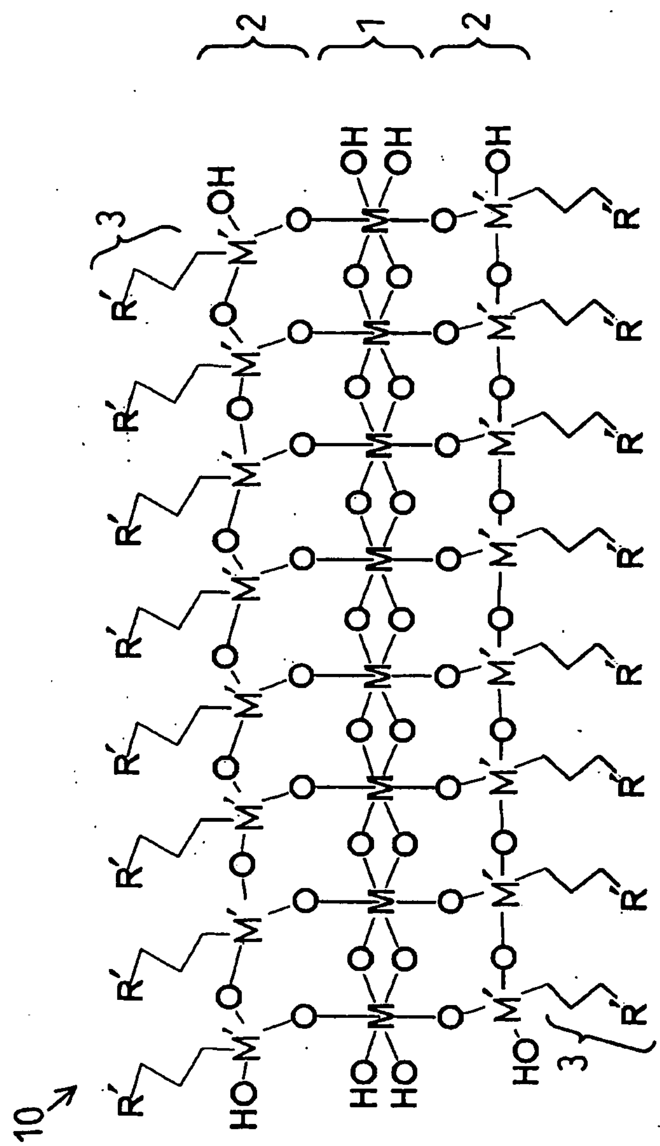
an octahedral structural layer made of octahedral structures whose central atom M is a second metallic atom; and

the layer organic-inorganic composite expressed by a general formula, $\{R_nM'O_{(4-n)/2}\}_x(MO_{z/2})(H_2O)_w$, wherein n is an integer of from 1 to 3, x is from 0.5 to 2.0, z is the valence number of the central atom M and is an integer of from 2 to 4, and w is the number of crystal water molecules and is an integer falling in a range of from {(z/2)-1} to (z+1)/2.

2. The paint composition set forth in claim 1, wherein the first metallic atom substituting for a part of the Si and making the central atom M′ is at least one atom selected from the group consisting of Al, Fe, P and Ti.

5000-5119

FIG. 1



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CONFIRMATION NO. 76

SERIAL NUMBER	FILING DATE	CLASS	GROUP ART UNIT	ATTORNEY DOCKE NO.
10/629,016	07/29/2003 RULE	428	1711	5000-5119

APPLICANTS

Masaaki Tani, Nagoya-shi, JAPAN;

Yoshiaki Fukushima, Aichi-ken, JAPAN;
Toshihisa Shimo, Kariya-shi, JAPAN;Hitotoshi Murase, Kariya-shi, JAPAN;

** CONTINUING DATA *************************

** FOREIGN APPLICATIONS ********************
JAPAN 2002-227787 08/05/2002

IF REQUIRED, FOREIGN FILING LICENSE GRANTED
** 10/28/2003

	STATE OR COUNTRY	SHEETS DRAWING	TOTAL CLAIMS	INDEPENDE CLAIMS
Foreign Priority claimed ☐ yes ☐ no 35 USC 119 (a-d) conditions met ☐ yes ☐ no ☐ Met after Allowance Verified and Acknowledged ______ Examiner's Signature ______ Initials	JAPAN	2	20	3

ADDRESS
27123
MORGAN & FINNEGAN, L.L.P.
3 WORLD FINANCIAL CENTER
NEW YORK , NY
10281-2101

TITLE
Paint composition, proces for producing wear-resistant coating film using the same ,and wear-resistant coating film comprising the same

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750	FEES: Authority has been given in Paper No. _________ to charge/credit DEPOSIT ACCOUNT No. _________ for following:	☐ All Fees ☐ 1.16 Fees (Filing) ☐ 1.17 Fees (Processing Ext. of time ☐ 1.18 Fees (Issue) ☐ Other ____________ ☐ Credit

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=> display history full l1-


     FILE 'HCAPLUS'
L1          8983 SEA TANI ?/AU
L2         13480 SEA FUKUSHIMA ?/AU
L3           843 SEA SHIMO ?/AU
L4             1 SEA L1 AND L2 AND L3
                 SEL L4 1 RN

     FILE 'REGISTRY'
L5             6 SEA (546-68-9/BI OR 2530-85-0/BI OR 4369-14-6/BI OR

     FILE 'LCA'
L6          7647 SEA (FILM? OR THINFILM? OR LAYER? OR OVERLAY? OR
                 OVERLAID? OR LAMIN? OR LAMEL? OR SHEET? OR LEAF? OR
                 FOIL? OR COAT? OR TOPCOAT? OR OVERCOAT? OR VENEER? OR
                 SHEATH? OR COVER? OR ENVELOP? OR ENCAS? OR ENWRAP? OR
                 OVERSPREAD?)/BI,AB

     FILE 'HCA'
L7          1775 SEA TETRAHED?(2A)L6
L8          2209 SEA OCTAHED?(2A)L6

     FILE 'REGISTRY'
L9          5151 SEA (C(L)H(L)O(L)TI)/ELS (L) 4/ELC.SUB
L10         1123 SEA L9 AND NO RSD/FA

     FILE 'HCA'
L11        23787 SEA L10 OR (TITANIUM# OR TI OR TITANATE#)(2A)(ALKOXIDE#
                 OR METHOXIDE# OR ETHOXIDE# OR PROPOXIDE# OR ISOPROPOXIDE#
                  OR BUTOXIDE# OR ISOBUTOXIDE#) OR TI(A)(OME OR OET OR
                 OPR OR OBU OR OIPR OR OIBU OR OSBU OR OTBU OR O(2A)(PR
                 OR BU OR IPR OR IBU OR SBU OR TBU))

     FILE 'REGISTRY'
L12            3 SEA L5 AND SI/ELS

     FILE 'HCA'
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L13        9533 SEA L12
L14             QUE SILICON OR SI
L15           3 SEA L7 AND L11
L16           4 SEA L8 AND L11
L17           1 SEA (L15 OR L16) AND L13
L18           3 SEA (L15 OR L16) AND L14
L19       64401 SEA TETRAHED?
L20       69331 SEA OCTAHED?
                E COATINGS/CV
L21       43471 SEA "COATING(S)"/CV OR COATINGS/CV
                E COATING MATERIALS/CV
L22      255494 SEA "COATING MATERIALS"/CV
                E COATING PROCESS/CV
L23      116098 SEA "COATING PROCESS"/CV
L24           6 SEA L19 AND (L21 OR L22 OR L23) AND L11
L25           6 SEA L20 AND (L21 OR L22 OR L23) AND L11
L26           1 SEA (L24 OR L25) AND L13
L27           8 SEA (L24 OR L25) AND L14
L28         130 SEA L19 AND L11
L29           4 SEA L28 AND L13
L30          55 SEA L28 AND L14
L31         160 SEA L20 AND L11
L32           1 SEA L31 AND L13
L33          31 SEA L31 AND L14
L34          17 SEA L30 AND L33
L35           3 SEA L34 AND (L21 OR L22 OR L23)
L36           9 SEA L34 AND L6
L37       82368 SEA PAINT?
L38           1 SEA L30 AND L37
L39           1 SEA L33 AND L37
L40         249 SEA L37 AND L11
L41           1 SEA L40 AND L19
L42           1 SEA L40 AND L20

     FILE 'REGISTRY'
L43           1 SEA L5 AND AL/ELS

     FILE 'HCA'
L44       55299 SEA L43 OR ALCL3
L45      137124 SEA (ALUMINUM# OR AL OR IRON# OR FE OR PHOSPHORUS# OR
                P)(2A)(SUBST? OR INTERCALAT? OR DOPE# OR DOPANT? OR
                DOPING#)
L46           2 SEA L30 AND L44
L47           0 SEA L30 AND L45
L48           1 SEA L33 AND L44
L49           0 SEA L33 AND L45
L50         130 SEA L11 AND L19
L51         160 SEA L11 AND L20
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L52           2 SEA L50 AND L44
L53           1 SEA L51 AND L44
L54           0 SEA L50 AND L45
L55           0 SEA L51 AND L45
L56          21 SEA L15 OR L16 OR L17 OR L18 OR L24 OR L25 OR L26 OR L27
                OR L29 OR L32 OR L35 OR L36 OR L38 OR L39 OR L41 OR L42
                OR L46 OR L48 OR L52 OR L53
L57           8 SEA L34 NOT L56
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=> file hca
FILE 'HCA'

=> d l56 1-21 cbib abs hitstr hitind

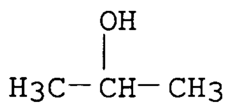
L56 ANSWER 1 OF 21 HCA COPYRIGHT 2005 ACS on STN
140:173266 Supercritical fluid-assisted deposition of materials on semiconductor substrates. Xu, Chongying; Baum, Thomas H.; Korzenski, Michael B. (USA). U.S. Pat. Appl. Publ. US 2004023453 A1 20040205, 15 pp., Cont.-in-part of U.S. Ser. No. 303,479. (English). CODEN: USXXCO. APPLICATION: US 2003-632009 20030731. PRIORITY: US 2001-PV345738 20011231; US 2002-303479 20021125.

AB Supercrit. fluid-assisted deposition of materials on substrates, such as semiconductor substrates for integrated circuit device manuf. The deposition is effected using a supercrit. fluid-based compn. contg. the precursor(s) of the material to be deposited on the substrate surface. Such approach permits use of precursors that otherwise would be wholly unsuitable for deposition applications, as lacking requisite volatility and transport characteristics for vapor phase deposition processes.

IT **546-68-9, Titanium** (IV) **isopropoxide**
3087-36-3, Titanium (IV) **ethoxide**
3087-39-6 5593-70-4, Titanium (IV) n-**butoxide**
(deposition precursor; supercrit. fluid-assisted deposition of materials on semiconductor substrates)

RN 546-68-9 HCA

CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



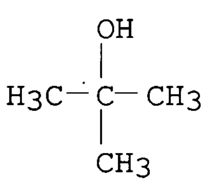
●1/4 Ti(IV)

RN 3087-36-3 HCA
CN Ethanol, titanium(4+) salt (9CI) (CA INDEX NAME)

H_3C-CH_2-OH

●1/4 Ti(IV)

RN 3087-39-6 HCA
CN 2-Propanol, 2-methyl-, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

RN 5593-70-4 HCA
CN 1-Butanol, titanium(4+) salt (9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-OH$

●1/4 Ti(IV)

IC ICM H01L021-8238
NCL 438202000
CC 76-2 (Electric Phenomena)
IT **Coating process**

(supercrit. fluid assisted; supercrit. fluid-assisted deposition of materials on semiconductor substrates)

IT 11105-01-4, **Silicon** nitride oxide 12033-62-4, Tantalum nitride (TaN) 12033-89-5, **Silicon** nitride, uses 12058-38-7, Tungsten nitride (WN) 25583-20-4, Titanium nitride (TiN) 37245-81-1, Molybdenum nitride 37271-26-4, Titanium nitride oxide 50816-03-0, Tungsten nitride oxide 52036-92-7, Tantalum nitride oxide 141325-59-9, Molybdenum nitride oxide
(barrier material; supercrit. fluid-assisted deposition of materials on semiconductor substrates)

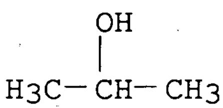
IT 142-71-2, Acetic acid, copper(2+) salt 544-19-4, Formic acid, copper(2+) salt **546-68-9, Titanium** (IV) **isopropoxide** 595-89-1, Tetraphenyl lead 603-33-8, Triphenyl bismuth 865-35-0, Tantalum (V) methoxide 2218-80-6, Cyclohexanebutanoic acid, copper(2+) salt **3087-36-3, Titanium** (IV) **ethoxide 3087-39-6** 3275-24-9, Tetrakis(dimethylamino)titanium 4419-47-0, Tetrakis(diethylamino)titanium **5593-70-4, Titanium** (IV) n-**butoxide** 6074-84-6, Tantalum (V) ethoxide 7803-62-5, Silane, reactions 12154-84-6, Iridium, [(1,2,5,6-.eta.)-1,5-cyclooctadiene](2,4-pentanedionato-.kappa.O,.kappa.O')- 13053-54-8, Ethanol, 2,2,2-trifluoro-, tantalum(5+) salt 13395-16-9 13939-06-5, Molybdenum hexacarbonyl (Mo(CO)6) 14040-05-2, Copper, bis(2,2,6,6-tetramethyl-3,5-heptanedionato-.kappa.O,.kappa.O')- 14040-11-0 14221-02-4, Tetrakis(triphenylphosphine)platinum 14781-45-4, Copper, bis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-.kappa.O,.kappa.O')-, (SP-4-1)- 14951-50-9, Dimethylgold(III)acetylacetonate 15243-33-1, Ruthenium carbonyl (Ru3(CO)12) 15443-06-8, Copper, bis(1-phenyl-1,3-pentanedionato-.kappa.O,.kappa.O')- 17653-77-9, Bis(2,6-dimethyl-3,5-heptanedionato)copper 18165-85-0, tert-Butylsilane 18206-43-4, Copper, pentafluorophenyl- 18827-81-1, Iridium, dodecacarbonyltetra-, **tetrahedro** 19824-59-0, Pentakis(dimethylamino)tantalum 20219-33-4, Tantalum, tetraethoxy(2,4-pentanedionato-.kappa.O,.kappa.O')-, (OC-6-22)- 28356-46-9, Ethanedioic acid, copper(2+) salt (2:1) 41612-46-8, Iridium, [5,5'-bibicyclo[2.2.1]hept-2-ene]-6,6'-diyl[(2,3,5,6-.eta.)-bicyclo[2.2.1]hepta-2,5-diene](2,4-pentanedionato-.kappa.O,.kappa.O')-, stereoisomer 53513-40-9, Copper carbonyl chloride 69701-39-9, Copper, bis(2,2,7-trimethyl-3,5-octanedionato-O,O')- 86233-74-1, Copper, [(1,2,5,6-.eta.)-1,5-cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-.kappa.O,.kappa.O')- 89989-39-9, Copper, (.eta.5-2,4-cyclopentadien-1-yl)(trimethylphosphine)- 94442-22-5, Trimethylmethylcyclopentadienyl platinum 102629-25-4, Copper, bis(4,4,4-trifluoro-1-phenyl-1,3-butanedionato-O,O')-, (SP-4-1)- 139566-53-3 142277-08-5, Copper, [(1,2,5,6-.eta.)-1,5-dimethyl-1,5-cyclooctadiene](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-

.kappa.O,.kappa.O')- 177279-28-6, Silver, [(.eta.2-ethenyl)triethylsilane](1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-O,O')- 181418-64-4, Tris(2,2,6,6-tetramethyl-3,5-heptanedionato)titanium 192817-15-5, Copper, (1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-.kappa.O,.kappa.O')[(3,4-.eta.)-2-methyl-1-hexen-3-yne]- 197842-49-2, Tantalum tetraethoxide 219723-09-8 284468-51-5, Ethanamine, N-methyl-, tantalum(5+) salt 329735-79-7, Ruthenium, [(1,2,5,6-.eta.)-1,5-cyclooctadiene]bis(2,2,6,6-tetramethyl-3,5-heptanedionato-.kappa.O,.kappa.O')- 593279-11-9, Copper, bis(6-methyl-2,4-heptanedionato-.kappa.O,.kappa.O')-, (SP-4-2)-
(deposition precursor; supercrit. fluid-assisted deposition of materials on semiconductor substrates)

L56 ANSWER 2 OF 21 HCA COPYRIGHT 2005 ACS on STN
140:154274 Synthesis of transparent Ti-containing mesoporous silica thin film materials and their unique photocatalytic activity for the reduction of CO2 with H2O. Shioya, Yasushi; Ikeue, Keita; Ogawa, Makoto; Anpo, Masakazu (Graduate School of Engineering, Department of Applied Chemistry, Osaka Prefecture University, Sakai, Osaka, 599-8531, Japan). Applied Catalysis, A: General, 254(2), 251-259 (English) 2003. CODEN: ACAGE4. ISSN: 0926-860X. Publisher: Elsevier Science B.V..

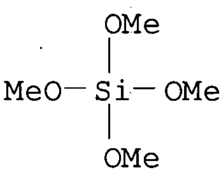
AB The transparent Ti-contg. mesoporous silica thin film materials having two different types of hexagonal and cubic pore structures with a thickness of about 50 .mu.m and a lateral size of a few centimeters were successfully synthesized by the solvent evapn. method from tetramethoxysilane (TMOS), vinyltrimethoxysilane (VTMOS), **titanium** tetra(iso-**propoxide**) (TIP), and octadecyltrimethylammonium chloride (C18TAC). The films were converted to Ti-contg. nanoporous silica thin films by subsequent calcinations in air at 823 K, while the highly ordered mesostructures and macroscopic morphol. were retained after the surfactant removal by calcination. The films with hexagonal and cubic symmetry were obtained by changing the compn. of the starting mixts. Various spectroscopic measurements of these films clearly showed that Ti ions are present in the silica networks as a **tetrahedrally** coordinated Ti-oxide species with a high dispersion state. Thus, developed transparent Ti-contg. thin films were used as photocatalysts for the redn. of CO2 with H2O to evaluate their unique and high photocatalytic activity. UV irradn. of these films in the presence of CO2 and H2O led to the formation of CH4 and CH3OH as well as CO and O2 as minor products, their yields increasing linearly against irradn. time, indicating that these films operate as efficient photocatalysts to proceed such a difficult reaction catalytically at 323 K. Furthermore, the films having hexagonal pore structure exhibited higher photocatalytic activity than the Ti-MCM-41 powd. catalyst even with the same pore

structure.
IT 546-68-9, **Titanium** tetra(iso-**propoxide**)
681-84-5, Tetramethoxysilane
(prepn. of transparent Ti-contg. mesoporous silica thin film photocatalysts with hexagonal and cubic pore structures)
RN 546-68-9 HCA
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

RN 681-84-5 HCA
CN Silicic acid (H4SiO4), tetramethyl ester (8CI, 9CI) (CA INDEX NAME)



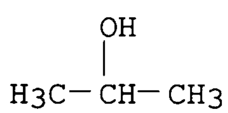
CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 67
IT 112-03-8, Octadecyltrimethylammonium chloride **546-68-9**, **Titanium** tetra(iso-**propoxide**) **681-84-5**, Tetramethoxysilane 2768-02-7, Vinyltrimethoxysilane
(prepn. of transparent Ti-contg. mesoporous silica thin film photocatalysts with hexagonal and cubic pore structures)
IT 7440-32-6D, Titanium, oxides, **tetrahedrally** coordinated in silica network 52337-09-4, Silicon titanium oxide
(synthesis of transparent Ti-contg. mesoporous silica thin film with hexagonal and cubic pore structures and their photocatalytic activity for redn. of CO2 with H2O)

L56 ANSWER 3 OF 21 HCA current application
140:129902 Organic-inorganic composite **paint** compositions for wear-resistant **coating films.** Tani, Masaaki; Fukushima, Yoshiaki; Shimo, Toshihisa; Murase, Hitotoshi (Japan). U.S. Pat. Appl. Publ. US 2004022706 A1 20040205, 14 pp. (English). CODEN: USXXCO. APPLICATION: US 2003-629016 20030729. PRIORITY: JP 2002-227787 20020805.

AB A **paint** compn. includes a **layer** org.-inorg. composite, and **titanium alkoxide** in an amt. of from 1 to 50 parts with respect to the **layer** org.-inorg. composite taken as 100 parts. The **layer** org.-inorg. composite is composed of a **laminated** substance. The **laminated** substance includes a **tetrahedral** structural **layer** and an **octahedral** structural **layer**. The **tetrahedral** structural **layer** is made of **tetrahedral** structures whose central atom is **Si** or a first metallic atom substituting for a part the **Si**, at least a part of the central atom covalent-bonded to an org. group involving or free from a polymerizable functional group. The **octahedral** structural **layer** is made of **octahedral** structures whose central atom is a second metallic atom.

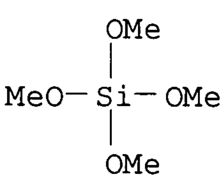
IT **546-68-9DP, Titanium isopropoxide,** reaction products with 3-methacryloxypropyltrimethoxy silane **681-84-5DP,** Tetramethoxy silane, reaction products with methacrylic titanosilicate **2530-85-0DP,** 3-Methacryloxy propyl trimethoxy silane, reaction products with **titanium isopropoxide 4369-14-6DP,** 3-Acryloxy propyl trimethoxy silane, reaction products with aluminum chloride hexahydrate **7784-13-6DP,** Aluminum chloride hexahydrate, reaction products with 3-acryloxypropyl trimethoxy silane
(org.-inorg. composite **paint** compns. for wear-resistant **coating films**)

RN 546-68-9 HCA
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)

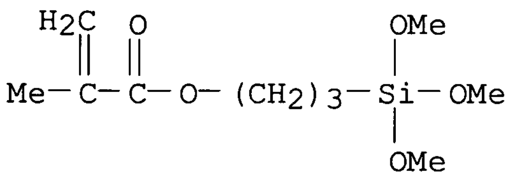


● 1/4 Ti(IV)

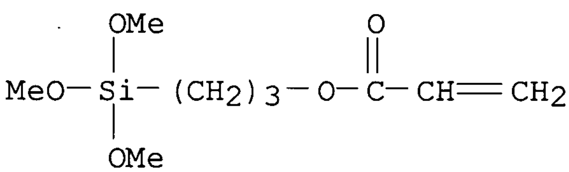
RN 681-84-5 HCA
CN Silicic acid (H4SiO4), tetramethyl ester (8CI, 9CI) (CA INDEX NAME)



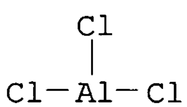
RN 2530-85-0 HCA
CN 2-Propenoic acid, 2-methyl-, 3-(trimethoxysilyl)propyl ester (9CI) (CA INDEX NAME)



RN 4369-14-6 HCA
CN 2-Propenoic acid, 3-(trimethoxysilyl)propyl ester (9CI) (CA INDEX NAME)



RN 7784-13-6 HCA
CN Aluminum chloride (AlCl3), hexahydrate (9CI) (CA INDEX NAME)



● 6 H_2O

IC ICM B05D001-36
NCL 423001000; 427402000
CC 42-10 (Coatings, Inks, and Related Products)
ST org inorg composite **paint** wear resistance **coating film**
IT **Coating materials**
(abrasion-resistant; org.-inorg. composite **paint** compns. for wear-resistant **coating films**)
IT **Titanates**
(**alkoxides**; org.-inorg. composite **paint** compns. for wear-resistant **coating films**)
IT Hybrid organic-inorganic materials
(**layered**; org.-inorg. composite **paint** compns. for wear-resistant **coating films**)

IT **Paints**
(org.-inorg. composite **paint** compns. for wear-resistant **coating films**)

IT Polycarbonates, miscellaneous
(substrate; org.-inorg. composite **paint** compns. for wear-resistant **coating films**)

IT Metal **alkoxides**
(**titanium**; org.-inorg. composite **paint** compns. for wear-resistant **coating films**)

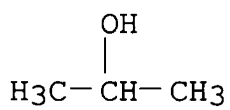
IT **546-68-9DP, Titanium isopropoxide,** reaction products with 3-methacryloxypropyltrimethoxy silane **546-68-9DP,** Titanium tetraisopropoxide, reaction products with methacrylic titanosilicate **681-84-5DP,** Tetramethoxy silane, reaction products with methacrylic titanosilicate **2530-85-0DP,** 3-Methacryloxy propyl trimethoxy silane, reaction products with **titanium isopropoxide** **4369-14-6DP,** 3-Acryloxy propyl trimethoxy silane, reaction products with aluminum chloride hexahydrate **7784-13-6DP,** Aluminum chloride hexahydrate, reaction products with 3-acryloxypropyl trimethoxy silane 7791-18-6DP, Magnesium chloride hexahydrate, reaction products with 3-methacryloxypropyltrimethoxy silane
(org.-inorg. composite **paint** compns. for wear-resistant **coating films**)

L56 ANSWER 4 OF 21 HCA COPYRIGHT 2005 ACS on STN

138:279461 Chemical approach using tailored liquid sources for traditional and novel ferroelectric thin films. Kato, Kazumi; Suzuki, Kazuyuki; Fu, Desheng; Nishizawa, Kaori; Miki, Takeshi (National Institute of Advanced Industrial Science and Technology, Nagoya, 463-8560, Japan). Japanese Journal of Applied Physics, Part 1: Regular Papers, Short Notes & Review Papers, 41(11B), 6829-6835 (English) 2002. CODEN: JAPNDE. Publisher: Japan Society of Applied Physics.

AB The Ca-Bi-Ti and Sr-Bi-**Ti** complex **alkoxide** solns. were used as tailored liq. sources for synthesis of a series of novel Bi-based layer-structured perovskite thin films with the no., n, of oxygen **octahedra** from 3 to 5. The complex alkoxide solns. had similar local structures, of which the stability for the partial hydrolysis was important to suppress compositional deviation in the resultant thin films. The Ca-contg. thin films had the characteristic well-developed columnar structure which was distinct from the refractory stacking-grain structure of the Sr-contained thin films. The relationship between the lattice consts. and the no. of oxygen **octahedra**, n, confirmed that the series of thin films prepd. using the alkoxide complex solns. had intentionally designed layer structure. Addnl., the dielec. and ferroelec. properties of the thin films were confirmed to depend on

the A-site cations and the value of n.
IT **546-68-9**, Titanium tetraisopropoxide
(chem. approach using tailored liq. sources for traditional and novel ferroelec. thin films)
RN 546-68-9 HCA
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 76-8 (Electric Phenomena)
IT **Coating process**
(spin; chem. approach using tailored liq. sources for traditional and novel ferroelec. thin films)
IT **546-68-9**, Titanium tetraisopropoxide 2914-17-2, Calcium ethoxide 2914-18-3, Strontium ethoxide 15049-66-8, Bismuth triethoxide 28099-67-4, Calcium methoxyethoxide 59664-68-5, Strontium bis(2-methoxyethoxide)
(chem. approach using tailored liq. sources for traditional and novel ferroelec. thin films)
IT 7440-21-3, **Silicon**, processes
(substrate; chem. approach using tailored liq. sources for traditional and novel ferroelec. thin films)

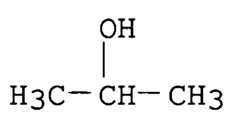
L56 ANSWER 5 OF 21 HCA COPYRIGHT 2005 ACS on STN
138:45478 Controlled coating of high surface area silica with titania overlayers by atomic layer deposition. Keranen, J.; Iiskola, E.; Guimon, C.; Auroux, A.; Niinisto, L. (Institut de Recherches sur la Catalyse, CNRS, Villeurbanne, F-69626, Fr.). Studies in Surface Science and Catalysis, 143(Scientific Bases for the Preparation of Heterogeneous Catalysts), 777-785 (English) 2002. CODEN: SSCTDM. ISSN: 0167-2991. Publisher: Elsevier Science B.V..
AB At. layer deposition (ALD) was applied to prep. highly dispersed titania/silica support materials by chemisorption of volatilized **titanium**(IV) **isopropoxide** on silica followed by an oxygen treatment. The practical temp. range for controlled precursor adsorption was obsd. to be between 110 and 180.degree.C as examd. by chem. anal. and inert atm. DRIFTS measurements. The surface modification was extented up to a monolayer coverage of titania by consecutive precursor binding - calcination cycles. The ALD TiO_2/SiO_2 samples maintained the high surface area and porosity as well the amorphous nature of the support even at high loadings.

At low coverage, titania was present in isolated **tetrahedral** units whereas at greater loadings, the coordination of titanium increased up to six-fold as suggested by UV-Vis DRS. Small titania particles (d < 3 nm) were obsd. by TEM after five ALD cycles (.apprx.5.1 Ti atoms/nm2support). However, no crystallites were detected by XRD even after seven ALD cycles (.apprx.7.0 Ti atoms/nm2support). Moreover, the uniformity and high relative dispersion of the titania species by formation of strong Ti-O-**Si** bonds was maintained even after several ALD cycles as probed by XPS. The importance of the prepn. mode was illustrated by comparing the ALD-dispersed titania/silica to a TiO_2-SiO_2 mech. mixt.

IT **546-68-9**, Titanium tetraisopropoxide
(controlled coating of high surface area silica with titania overlayers by at. layer deposition)

RN 546-68-9 HCA

CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 66, 75

IT Catalysts
Chemisorption
Coating process
Particle size
Porosity
Surface area
Surface structure
(controlled coating of high surface area silica with titania overlayers by at. layer deposition)

IT **546-68-9**, Titanium tetraisopropoxide 7782-44-7, Oxygen, reactions
(controlled coating of high surface area silica with titania overlayers by at. layer deposition)

L56 ANSWER 6 OF 21 HCA COPYRIGHT 2005 ACS on STN

136:239774 Chemical processing and characterization of ferroelectric thin films of bismuth-based layer-structured perovskite $CaBi_4Ti_4O_{15}$ with the **octahedron** number of 4. Kato, Kazumi; Suzuki,

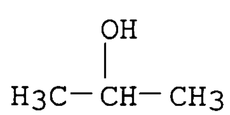
Kazuyuki; Nishizawa, Kaori; Miki, Takeshi (National Institute of Advanced Industrial Science and Technology, Nagoya, 462-8510, Japan). Integrated Ferroelectrics, 36(1-4), 321-329 (English) 2001. CODEN: IFEREU. ISSN: 1058-4587. Publisher: Gordon & Breach Science Publishers.

AB CaBi4Ti4O15 (CBTi144) thin films were prepd. by spin-coating a precursor soln. of metal alkoxides. As-deposited thin films began crystn. below 550.degree.C and reached full crystallinity of a single phase of layered perovskite at 650.degree.C via rapid thermal annealing in oxygen. 650.degree.C-annealed CBTi144 thin film showed random orientation and had a columnar structure on Pt-passivated **Si** substrate. The dielec. const. and loss factor were 300 and 0.033, resp., at 100 kHz. The thin film exhibited P-E hysteresis loops. The remanent polarization (Pr) and coercive elec. field (Ec) were 6.0 .mu.C/cm2 and 78.7 kV/cm, resp., at 9 V. The thin film showed good endurance properties against no. of switching cycles.

IT **546-68-9**, Titanium tetraisopropoxide
(chem. processing and characterization of ferroelec. thin films of bismuth-based layer-structured perovskite CaBi4Ti4O15 with the **octahedron** no. of 4)

RN 546-68-9 HCA

CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 76-8 (Electric Phenomena)

IT Calcination
Dielectric constant
Dielectric hysteresis
Dielectric loss
Dielectric polarization
Ferroelectric films
Ferroelectricity
Hydrolysis
Microstructure
Rapid thermal annealing
(chem. processing and characterization of ferroelec. thin films of bismuth-based layer-structured perovskite CaBi4Ti4O15 with the **octahedron** no. of 4)

IT **Coating process**

(spin; chem. processing and characterization of ferroelec. thin films of bismuth-based layer-structured perovskite CaBi4Ti4O15 with the **octahedron** no. of 4)

IT 12297-31-3P, Bismuth calcium titanium oxide Bi4CaTi4O15
(chem. processing and characterization of ferroelec. thin films of bismuth-based layer-structured perovskite CaBi4Ti4O15 with the **octahedron** no. of 4)

IT **546-68-9**, Titanium tetraisopropoxide 7440-70-2, Calcium, reactions 15049-66-8, Bismuth triethoxide
(chem. processing and characterization of ferroelec. thin films of bismuth-based layer-structured perovskite CaBi4Ti4O15 with the **octahedron** no. of 4)

IT 7440-06-4, Platinum, processes 7631-86-9, Silica, processes 13463-67-7D, Titania, oxygen-deficient, processes
(film; chem. processing and characterization of ferroelec. thin films of bismuth-based layer-structured perovskite CaBi4Ti4O15 with the **octahedron** no. of 4)

IT 7440-21-3, **Silicon,** processes
(substrate; chem. processing and characterization of ferroelec. thin films of bismuth-based layer-structured perovskite CaBi4Ti4O15 with the **octahedron** no. of 4)

L56 ANSWER 7 OF 21 HCA COPYRIGHT 2005 ACS on STN

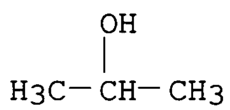
135:201102 Transparent self-standing films of titanium-containing nanoporous silica. Ogawa, Makoto; Ikeue, Keita; Anpo, Masakazu (PRESTO Japan Science and Technology Corporation (JST) Department of Earth Sciences, Waseda University, Shinjuku-ku Tokyo, 169-8050, Japan). Chemistry of Materials, 13(9), 2900-2904 (English) 2001. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.

AB Transparent self-standing films of Ti-contg. (Ti/Si ratio of 1/50) silica-surfactant mesostructured materials, having a thickness of ca. 50 .mu.m and a lateral size of a few centimeters, were synthesized by the solvent evapn. method from tetramethoxysilane, vinyltrimethoxysilane, Ti tetraisopropoxide, and octadecyltrimethylammonium chloride. The films were converted to Ti-contg. nanoporous silica films by subsequent calcination in air at 550.degree., while their highly ordered mesostructures and macroscopic morphol. were retained after the surfactant removal. Ti-contg. nanoporous silica films with hexagonal and cubic symmetry were obtained by changing the compn. of the starting mixts. The resulting materials possess a large surface area (.apprxeq.900 m2/g) as evidenced by N2 adsorption/desorption isotherms. The Ti ions exist in the silica network as a **tetrahedrally** coordinated species. UV irradn. of the Ti-contg. nanoporous silica film in the presence of CO2 and H2O led to the evolution of CH4 and CH3OH, indicating the photocatalytic reactivity of the present material.

IT **546-68-9**, Titanium tetraisopropoxide **681-84-5**,

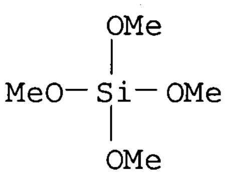
Tetramethoxysilane
(in prepn. of transparent self-standing films of titanium-contg. nanoporous silica)

RN 546-68-9 HCA
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

RN 681-84-5 HCA
CN Silicic acid (H4SiO4), tetramethyl ester (8CI, 9CI) (CA INDEX NAME)



CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 57
IT 112-03-8, Octadecyltrimethylammonium chloride **546-68-9**, Titanium tetraisopropoxide **681-84-5**, Tetramethoxysilane 2768-02-7, Vinyltrimethoxysilane
(in prepn. of transparent self-standing films of titanium-contg. nanoporous silica)

L56 ANSWER 8 OF 21 HCA COPYRIGHT 2005 ACS on STN
135:156483 Effect of silica additive on the anatase-to-rutile phase transition. Okada, Kiyoshi; Yamamoto, Nobuo; Kameshima, Yoshikazu; Yasumori, Atsuo; MacKenzie, Kenneth J. D.; Condrate, R. A. (Department of Metallurgy and Ceramics Science, Tokyo Institute of Technology, Tokyo, 152-8552, Japan). Journal of the American Ceramic Society, 84(7), 1591-1596 (English) 2001. CODEN: JACTAW. ISSN: 0002-7820. Publisher: American Ceramic Society.
AB The effect of SiO2 addn. on the anatase-to-rutile phase transition was investigated by DTA, XRD, FTIR, and XPS. TiO2 xerogels contg. SiO2 up to 20 mol% were prepd. by mixing and hydrolyzing titanium tetraisopropoxide (TTIP) and tetraethylorthosilicate (TEOS) with HNO3 as a catalyst. With increased amts. of SiO2 in the xerogels, the following results were obtained: (1) the crystn. temp. of

anatase increased from 415.degree.C in pure TiO2 to 609.degree.C in 20-mol%-SiO2-contg. xerogel in the DTA curves; (2) the formation temp. of rutile, according to quant. XRD anal., increased with increased SiO2 content up to 5 mol% SiO2 but became const. at higher SiO2 contents; (3) the crystallinity of anatase became lower; and (4) the lattice parameter a of the anatase decreased slightly, but the parameter c decreased greatly up to 20 mol% SiO2. Although the added **silicon** atoms were considered from these results to be incorporated into the amorphous TiO2 and anatase structures, the 29Si MAS NMR spectra of the xerogels contg. 10 mol% SiO2 showed only **tetrahedral silicon**, with no indication of **silicon** in **octahedral** coordination. When calcined at higher temps., the xerogel showed polymn. of the SiO4 **tetrahedra** in the NMR spectra and the **Si**-O-**Si** vibration in the FTIR spectra. The chem. compn. of the xerogel surfaces, measured using XPS, showed increased SiO2 content with increased calcining temp., indicating the expulsion of **silicon** from inside the particles to form an amorphous SiO2 surface **layer**. The formation of this amorphous SiO2 surface **layer** was considered to be important in retarding the anatase-to-rutile phase transition by suppressing diffusion between anatase particles in direct contact and limiting their ability to act as surface nucleation sites for rutile. These effects of **silicon** addns. were similar to those obsd. in the .gamma.-Al2O3-to-.alpha.-Al2O3 transition.

IT **53339-36-9**, Titanium tetraisopropoxide homopolymer
(xerogels; effect of silica additive on anatase-to-rutile phase transition)

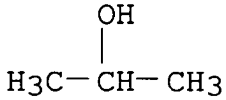
RN 53339-36-9 HCA

CN 2-Propanol, titanium(4+) salt, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 546-68-9

CMF C3 H8 O . 1/4 Ti



●1/4 Ti(IV)

CC 57-2 (Ceramics)

IT **53339-36-9**, Titanium tetraisopropoxide homopolymer
(xerogels; effect of silica additive on anatase-to-rutile phase

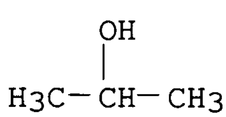
transition)

L56 ANSWER 9 OF 21 HCA COPYRIGHT 2005 ACS on STN
135:13447 Influence of the Ti precursor on the properties of Ti-pillared smectites. Vicente, M. A.; Banares-Munoz, M. A.; Toranzo, R.; Gandia, L. M.; Gil, A. (Departamento de Quimica Inorganica, Universidad de Salamanca, Salamanca, 37008, Spain). Clay Minerals, 36(1), 125-138 (English) 2001. CODEN: CLMIAF. ISSN: 0009-8558. Publisher: Mineralogical Society.

AB The pillaring of smectites (two saponites and a montmorillonite) with various Ti precursors was studied. The minerals were intercalated with classical titanium precursors, such as TiCl4 and **Ti(OEt)**4, and also with new precursors, such as solns. of Ti(OPri)4 in HOAc, or bis(ethylacetoacetato)diisopropoxytitanium (Ti(etacet)2(isop)2) in acetone. A complete characterization of the intercalated solids was carried out and a comparison of the properties of the solids as a function of the precursors used in the intercalation established. The influence of the severe conditions in which the intercalation with Ti oligomers is usually carried out (low pH and/or high temp.) on the properties of the intercalated solids was analyzed. Intercalation with TiCl4 and Ti(EtO)4 strongly affected the structure of the clays, not by acid attack on the **octahedral sheet**, but mainly by disaggregation of particles. Ti(OPri)4 is less aggressive for the clays, while Ti(etacet)2(isop)2 did not form pillared solids but organo-clays, and therefore was of no use as a pillaring agent. The solids were thermally stable up to 300.degree., showing a high sp. surface area.

IT **546-68-9DP**, Titanium tetraisopropoxide, pillared saponite and montmorillonite derivs. **3087-36-3DP**, Titanium tetraethoxide, pillared saponite and montmorillonite derivs.
(prepn. of smectites pillared with titanium precursors and effect on structure, thermal stability, and sp. surface area)

RN 546-68-9 HCA
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

RN 3087-36-3 HCA
CN Ethanol, titanium(4+) salt (9CI) (CA INDEX NAME)

H_3C-CH_2-OH

●1/4 Ti(IV)

CC 78-3 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75

IT **546-68-9DP,** Titanium tetraisopropoxide, pillared saponite and montmorillonite derivs. **3087-36-3DP,** Titanium tetraethoxide, pillared saponite and montmorillonite derivs. 7550-45-0DP, Titanium tetrachloride, pillared saponite and montmorillonite derivs.
(prepn. of smectites pillared with titanium precursors and effect on structure, thermal stability, and sp. surface area)

L56 ANSWER 10 OF 21 HCA COPYRIGHT 2005 ACS on STN

134:375257 A Novel Titanosilicate with MWW Structure. I. Hydrothermal Synthesis, Elimination of Extraframework Titanium, and Characterizations. Wu, Peng; Tatsumi, Takashi; Komatsu, Takayuki; Yashima, Tatsuaki (Division of Materials Science & Chemical Engineering Faculty of Engineering, Yokohama National University, Hodogaya-ku Yokohama, 240-8501, Japan). Journal of Physical Chemistry B, 105(15), 2897-2905 (English) 2001. CODEN: JPCBFK. ISSN: 1089-5647. Publisher: American Chemical Society.

AB A novel titanosilicate with MWW topol., Ti-MWW, was prepd. by an acid treatment on a corresponding **lamellar** precursor which is hydrothermally synthesized with the coexistence of B and Ti using piperidine (PI) or hexamethyleneimine (HM) as a structure-directing agent. The MWW precursor can be synthesized to have a **Si**/Ti ratio .gtoreq.10 when the **Si**/B ratio of the gel is maintained at 0.75. Both the materials synthesized using PI and HM exhibit the crystal form of thin platelets, while the latter shows a larger crystal size. Besides the **tetrahedral** Ti species, the precursor always contains the **octahedral** Ti species showing a UV-visible band at 260 nm, regardless of the Ti content. Calcination of the precursor results in a partial condensation of the **octahedral** Ti species to form the anatase phase, which is hardly removed by the acid treatment. MWW-type titanosilicate nearly free of both anatase and B, however, is successively prepd. by a cyclic treatment on the **lamellar** precursor, i.e., an acid treatment, subsequent calcination, and a further acid treatment. After evacuation at 773 K, the titanosilicate thus prepd. shows a characteristic IR band at 960 cm-1 not obsd. for the Ti-free sample. The intensity of the 960 cm-1 band increases linearly with the Ti content up to a level corresponding to

Si/Ti = 40, indicating the limitation of incorporating Ti into the framework of MWW by the present method.

IT **5593-70-4**, Tetrabutyl orthotitanate
(for hydrothermal prepn. of titanosilicate with MWW structure and with/without framework boron)

RN 5593-70-4 HCA

CN 1-Butanol, titanium(4+) salt (9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-OH$

●1/4 Ti(IV)

CC 78-4 (Inorganic Chemicals and Reactions)

IT **5593-70-4**, Tetrabutyl orthotitanate 7631-86-9, Cab-o-sil M7D, reactions
(for hydrothermal prepn. of titanosilicate with MWW structure and with/without framework boron)

L56 ANSWER 11 OF 21 HCA

134:346347 Preparation, characterization and photocatalytic properties of singly and doubly titania-modified mesoporous silicate MCM-41 by varying titanium precursors. Zheng, Shan; Gao, Lian; Zhang, Qinghong; Zhang, Weiping; Guo, Jingkun (State Key Laboratory of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, 200050, Peop. Rep. China). Journal of Materials Chemistry, 11(2), 578-583 (English) 2001. CODEN: JMACEP. ISSN: 0959-9428. Publisher: Royal Society of Chemistry.

AB A series of titania-modified MCM-41 have been synthesized from varying three kinds of titanium precursors [Ti(OBun)4, Ti(OBun)3(acac), Ti(OBun)2(acac)2] resp. and mesoporous mol. sieve MCM-41, in which titania existed as single or double **layers** (acac = acetylacetonate). The samples were characterized by powder x-ray diffraction (XRD), nitrogen adsorption-desorption at 77 K, 29Si MAS NMR, FTIR and Raman spectroscopy, as well as by solid state diffuse reflectance UV-VIS spectroscopy. The titanium precursor was cocondensed with the active silanol groups of MCM-41 via **Si** -O-Ti bonds and the resulting titania modified the mesopore walls of MCM-41 after hydrolysis and calcination. In the titania-modified MCM-41 samples, although the titania species were in an amorphous state and in **tetrahedral** coordination rather than **octahedral** coordination, which exists extensively in cryst. titania, they exhibited high photocatalytic activity for the photodecompn. of phenol and the photoredn. of Cr(VI) to Cr(III).

IT **5593-70-4**, **Titanium** tetra-n-**butoxide**

(prepn. and characterization and photocatalytic properties of mesoporous silicate MCM-41 titania-modified by varying titanium precursors)

RN 5593-70-4 HCA

CN 1-Butanol, titanium(4+) salt (9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-OH$

● 1/4 Ti(IV)

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT **5593-70-4, Titanium** tetra-n-**butoxide**
16902-59-3, Bis(Acetylacetonato)di-butoxytitanium 34794-90-6, (Acetylacetonato)tri-butoxytitanium
(prepn. and characterization and photocatalytic properties of mesoporous silicate MCM-41 titania-modified by varying titanium precursors)

L56 ANSWER 12 OF 21 HCA COPYRIGHT 2005 ACS on STN

134:50542 Integrated Experimental and Computational Methods for Structure Determination and Characterization of a New, Highly Stable Cesium Silicotitanate Phase, Cs2TiSi6O15 (SNL-A). Nyman, M.; Bonhomme, F.; Teter, D. M.; Maxwell, R. S.; Gu, B. X.; Wang, L. M.; Ewing, R. C.; Nenoff, T. M. (Catalysis and Chemical Technologies Department, Sandia National Laboratories, Albuquerque, NM, 87185, USA). Chemistry of Materials, 12(11), 3449-3458 (English) 2000. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.

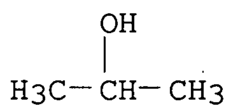
AB Exploratory hydrothermal synthesis in the system Cs2O-SiO2-TiO2 produced a new polymorph of Cs2TiSi6O15 (SNL-A), whose structure was detd. using a combination of exptl. and theor. techniques (29Si and 133Cs NMR, x-ray powder diffraction, and d. functional theory). SNL-A crystallizes in the monoclinic space group Cc with a 12.998(2), b 7.5014(3), c 15.156(3) .ANG., and .beta. 105.80(3).degree.. The SNL-A framework is an unbranched drier single-**layer** silicate with **silicon** **tetrahedra** and titanium **octahedra** that are linked in 3-, 5-, 6-, 7-, and 8-membered rings in three dimensions. SNL-A is distinctive from a previously reported C2/c polymorph of Cs2TiSi6O15 by orientation of the Si2O52- **layers** and by different ring geometries. Similarities and differences between the two structures are discussed. Other characterizations of SNL-A include TGA-DTA, Cs/**Si**/Ti elemental analyses, and SEM/EDS. Also, the chem. and radiation durability of SNL-A was studied in

interest of ceramic waste form applications. These studies show that SNL-A is durable in both radioactive and rigorous chem. environments. Finally, calcd. cohesive energies of the two Cs2TiSi6O15 polymorphs suggest that the Cc SNL-A phase (synthesized at 200.degree.) is energetically more favorable than the C2/c polymorph (synthesized at 1050.degree.).

IT **546-68-9**, **Titanium**(IV) **isopropoxide**
(reactant for hydrothermal prepn. of cesium silicotitanate (Cs2TiSi6O15, SNL-A) Cc polymorph)

RN 546-68-9 HCA

CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 78-6 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 71, 75

IT 78-10-4, Tetraethyl orthosilicate **546-68-9**, **Titanium**(IV) **isopropoxide** 21351-79-1, Cesium hydroxide (CsOH)
(reactant for hydrothermal prepn. of cesium silicotitanate (Cs2TiSi6O15, SNL-A) Cc polymorph)

L56 ANSWER 13 OF 21 HCA COPYRIGHT 2005 ACS on STN

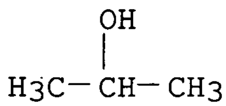
133:45686 Titanostannosilicates and preparation thereof. Nemeth, Laszlo; Lewis, Gregory J.; Rosin, Richard R. (UOP L.L.C., USA). U.S. US 6074624 A 20000613, 7 pp., Cont.-in-part of U.S. 5,780,654. (English). CODEN: USXXAM. APPLICATION: US 1998-109854 19980702. PRIORITY: US 1997-840531 19970422.

AB A new family of cryst. titanostannosilicate mol. sieves have been synthesized. These mol. sieves have a microporous three-dimensional framework of TiO2, SnO2 and SiO2 **tetrahedral** oxide units and are represented by the empirical formula: (TixSnySiz)O2 where x, y and z are the mole fractions of Ti, Sn, and Si, resp. These mol. sieves are active catalysts for the epoxidn. of olefins by peroxides such as hydrogen peroxide.

IT **546-68-9**, Titanium tetraisopropoxide **681-84-5**, Tetramethylorthosilicate **3087-36-3**, Titanium tetraethoxide **5593-70-4**, Titanium tetrabutoxide
(manuf. of titanostannosilicates for use as epoxidn. catalyst)

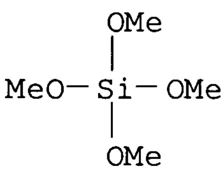
RN 546-68-9 HCA

CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

RN 681-84-5 HCA
CN Silicic acid (H4SiO4), tetramethyl ester (8CI, 9CI) (CA INDEX NAME)



RN 3087-36-3 HCA
CN Ethanol, titanium(4+) salt (9CI) (CA INDEX NAME)

H_3C-CH_2-OH

●1/4 Ti(IV)

RN 5593-70-4 HCA
CN 1-Butanol, titanium(4+) salt (9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-OH$

●1/4 Ti(IV)

IC ICM C01B039-06
NCL 423702000
CC 49-4 (Industrial Inorganic Chemicals)
Section cross-reference(s): 45
IT 78-10-4, Tetraethylorthosilicate **546-68-9**, Titanium tetraisopropoxide **681-84-5**, Tetramethylorthosilicate 1332-29-2, Tin oxide **3087-36-3**, Titanium tetraethoxide 4499-86-9, Tetrapropylammonium hydroxide **5593-70-4**,

Titanium tetrabutoxide 7631-86-9, Silica, processes 7722-84-1, Hydrogen peroxide, processes 13010-31-6D, Tetrapropylammonium, halides 13463-67-7, Titanium oxide (TiO2), processes
(manuf. of titanostannosilicates for use as epoxidn. catalyst)

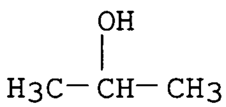
L56 ANSWER 14 OF 21 HCA COPYRIGHT 2005 ACS on STN
132:99713 Nanocrystalline TiO2 studied by optical, FTIR and X-ray photoelectron spectroscopy: correlation to presence of surface states. Kumar, P. M.; Badrinarayanan, S.; Sastry, M. (Materials Chemistry Division, National Chemical Laboratory, Pune, India). Thin Solid Films, 358(1,2), 122-130 (English) 2000. CODEN: THSFAP. ISSN: 0040-6090. Publisher: Elsevier Science S.A..

AB Nanophase TiO2 was synthesized in an org. medium by two different routes, yielding two different structural phases viz. rutile and anatase. These differences are reflected in the different characterization techniques used to study the nanoparticles. UV-visible spectroscopy shows absorption-peak related particle sizes of .apprx.2.5 nm and agrees with TEM ests. of 2.5-5.0 nm. Grazing incidence x-ray diffraction shows rutile and anatase phase with an **overlay** of Ti2O3 for the different routes considered. Differences in the nature of the transition from absorption plots not withstanding, a direct transition is confirmed. Photo-luminescence (PL) spectra for the two particulate structures shows prominent red shifted peaks at 314 nm and 399 nm, resp. (0.81 eV from the excitation), and also reveals vibrational features around the max. PL signal. In addn. a Ti3+ (PL) state is obsd. at 617.5 nm for both cases, a feature governed by the Auger process. FTIR studies reveal weak complex vibrations between the Ti-O oxide species and also addnl. unsatd. sites (Ti3+) through incorporation of (OH) groups, not otherwise seen in bulk TiO2. A surface consisting of 6Ti3+-OH for coordinative satn. (**octahedral** site), along with 4Ti4+-O (**tetrahedral**) is thus necessary. Grazing incidence x-ray diffraction studies shows the rutile phase of TiO2 and also a sub-oxide phase of Ti (Ti2O3). X-ray photoemission spectra (XPS) of thin **films** of TiO2 confirms the oxide phase and also the presence of sub-valence states. The XPS and FTIR spectra confirm the presence of adsorbed sites for coordinative satn. of sub-valence states (Ti2+, Ti3+), through hydroxyl incorporation. These sites are amplified as the particle size is reduced, opening avenues for addnl. coordination, leading to important applications. In this case, a Ti2O3 **overlay** sats. the surface of TiO2. Subtle differences are obsd. in the data vis-a-vis literature reports.

IT **546-68-9**, Tetra-isopropyl orthotitanate
(nanocryst. TiO2 studied by optical, FTIR and XPS: correlation to presence of surface states)

RN 546-68-9 HCA

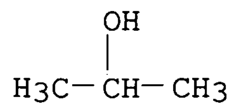
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

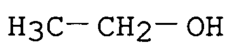
CC 73-3 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
IT **546-68-9**, Tetra-isopropyl orthotitanate 1344-54-3, Titanium sesquioxide
(nanocryst. TiO_2 studied by optical, FTIR and XPS: correlation to presence of surface states)
IT 7440-21-3, **Silicon**, uses
(substrate; nanocryst. TiO_2 studied by optical, FTIR and XPS: correlation to presence of surface states)

L56 ANSWER 15 OF 21 HCA COPYRIGHT 2005 ACS on STN
131:301204 Stannosilicate molecular sieves. Valencia, Susana Valencia; Canos, Avelino Corma (UOP LLC, USA). U.S. US 5968473 A 19991019, 5 pp. (English). CODEN: USXXAM. APPLICATION: US 1998-215815 19981218.
AB A new family of stannosilicate mol. sieves which have the zeolite beta structure are disclosed. These mol. sieves have a three dimensional framework structure composed of at least SnO_2 and SiO_2 **tetrahedral** oxide units (and optionally TiO_2 and GeO_2 units) and have an empirical formula of: $(Sn_xTi_ySi_{1-x-y-z}Ge_z)O_2$ where "x", "y" and "z" are the mole fractions of tin, titanium and germanium resp. A process for prepg. these mol. sieves is also presented along with processes for the selective oxidn. of org. compds. with peroxides using the mol. sieves as catalysts.
IT **546-68-9, Titanium isopropoxide**
3087-36-3 5593-70-4 7784-13-6, Aluminum chloride hexahydrate
(stannosilicate mol. sieves)
RN 546-68-9 HCA
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



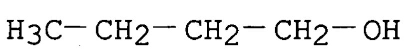
●1/4 Ti(IV)

RN 3087-36-3 HCA
CN Ethanol, titanium(4+) salt (9CI) (CA INDEX NAME)



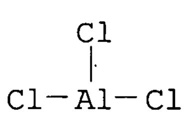
●1/4 Ti(IV)

RN 5593-70-4 HCA
CN 1-Butanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

RN 7784-13-6 HCA
CN Aluminum chloride (AlCl3), hexahydrate (9CI) (CA INDEX NAME)



●6 H_2O

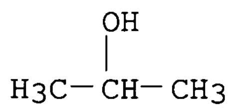
IC ICM C01B033-20
ICS C01B039-08
NCL 423702000
CC 49-4 (Industrial Inorganic Chemicals)
IT 247171-84-2P, **Silicon** tin oxide (Si0.99Sn0.01O2)
(stannosilicate mol. sieves)

IT 64-17-5, Ethanol, processes 66-40-0 77-98-5, Tetraethylammonium hydroxide 78-10-4 280-57-9, 1,4-Diazabicyclo[2.2.2]octane **546-68-9, Titanium isopropoxide** **3087-36-3** 3173-69-1 **5593-70-4** 7631-86-9, Silica, processes 7646-78-8, Tin tetrachloride, processes 7697-37-2, Nitric acid, processes 7722-84-1, Hydrogen peroxide, processes **7784-13-6**, Aluminum chloride hexahydrate 13463-67-7, Titanium oxide (TiO2), processes 14254-05-8 14800-26-1 73853-65-3 157858-56-5, Germanium oxide
(stannosilicate mol. sieves)

L56 ANSWER 16 OF 21 HCA COPYRIGHT 2005 ACS on STN
130:175131 Characterization of Ti/**Si** binary oxides prepared by the sol-gel method and their photocatalytic properties: the hydrogenation and hydrogenolysis of CH3CCH with H2O. Yamashita, Hiromi; Kawasaki, Shinichi; Ichihashi, Yuichi; Takeuchi, Masato; Harada, Masaru; Anpo, Masakazu; Louis, Catherine; Che, Michel (Department of Applied Chemistry, Osaka Prefecture University, Osaka, 599-8531, Japan). Korean Journal of Chemical Engineering, 15(5), 491-495 (English) 1998. CODEN: KJCHE6. ISSN: 0256-1115. Publisher: Korean Institute of Chemical Engineers.

AB Titanium-**silicon** (Ti/**Si**) binary oxides having different Ti content were prepd. by the sol-gel method and utilized as photocatalysts for the hydrogenation and hydrogenolysis of CH3CCH with H2O. The photocatalytic reactivity and selectivity of these catalysts were investigated as a function of the Ti content and it was found that the hydrogenolysis reaction (C2H6 formation) was predominant in regions of low Ti content, while the hydrogenation reaction (C3H6 formation) proceeded in regions of high Ti content. The in situ photoluminescence, diffuse reflectance absorption, FT-IR, XAFS (XANES and EXAFS), and XPS spectroscopic investigations of these Ti/**Si** binary oxides indicated that the titanium oxide species are highly dispersed in the SiO2 matrixes and exist in a **tetrahedral** coordination exhibiting a characteristic photoluminescence spectrum. The charge transfer excited state of the **tetrahedrally** coordinated titanium oxide species plays a significant role in the efficient photoreaction with a high selectivity for the hydrogenolysis of CH3CCH to produces mainly C2H6 and CH4, while the catalysts involving the aggregated **octahedrally** coordinated titanium oxide species show a high selectivity for the hydrogenation of CH3CCH to produce C3H6, being similar to reactions of the powd. TiO2 catalysts. The good parallel relationship between the yield of the photoluminescence and the specific photocatalytic reactivity of the Ti/**Si** binary oxides as a function of the Ti content clearly indicates that the high photocatalytic reactivity of the Ti/**Si** binary oxides having low Ti content is assocd. with the high reactivity of the charge transfer excited state of the isolated titanium oxide species

in **tetrahedral** coordination, [Ti3+-O-].bul..
IT **546-68-9, Titanium isopropoxide**
(photocatalytic properties of sol-gel prepd. Ti/**Si** binary oxides used for hydrogenation and hydrogenolysis of alkyne)
RN 546-68-9 HCA
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
ST titanium **silicon** binary oxide photocatalytic property; hydrogenation hydrogenolysis methylacetylene water titanium **silicon** oxide photocatalyst
IT Sol-gel processing
(**coating**; photocatalytic properties of sol-gel prepd. Ti/**Si** binary oxides used for hydrogenation and hydrogenolysis of alkyne)
IT Hydrogenation catalysts
Hydrogenolysis catalysts
Luminescence
Photolysis catalysts
XANES spectra
(photocatalytic properties of sol-gel prepd. Ti/**Si** binary oxides used for hydrogenation and hydrogenolysis of alkyne)
IT Alkynes
(photocatalytic properties of sol-gel prepd. Ti/**Si** binary oxides used for hydrogenation and hydrogenolysis of alkyne)
IT **Coating process**
(sol-gel; photocatalytic properties of sol-gel prepd. Ti/**Si** binary oxides used for hydrogenation and hydrogenolysis of alkyne)
IT 7631-86-9, Silica, properties 13463-67-7, Titania, properties
(photocatalytic properties of sol-gel prepd. Ti/**Si** binary oxides used for hydrogenation and hydrogenolysis of alkyne)
IT 74-84-0, Ethane, formation (nonpreparative) 115-07-1, Propylene, formation (nonpreparative)

(photocatalytic properties of sol-gel prepd. Ti/**Si** binary oxides used for hydrogenation and hydrogenolysis of alkyne)

IT 78-10-4, Tetraethylorthosilicate **546-68-9, Titanium isopropoxide**
(photocatalytic properties of sol-gel prepd. Ti/**Si** binary oxides used for hydrogenation and hydrogenolysis of alkyne)

IT 74-99-7, Methylacetylene 7732-18-5, Water, reactions
(photocatalytic properties of sol-gel prepd. Ti/**Si** binary oxides used for hydrogenation and hydrogenolysis of alkyne)

L56 ANSWER 17 OF 21 HCA COPYRIGHT 2005 ACS on STN

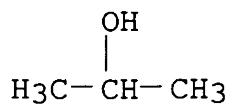
130:109916 Fluorescence Properties of 2,5-Bis(4-(diethylamino)phenyl)-1,3,4-oxadiazole Molecules Encapsulated in SiO2 and **Si**-Ti Binary Oxide Matrixes by the Sol-Gel Method. Zhang, Jinlong; Matsuoka, Masaya; Yamashita, Hiromi; Anpo, Masakazu (Department of Applied Chemistry College of Engineering, Osaka Prefecture University, Sakai Osaka, 599-8531, Japan). Langmuir, 15(1), 77-82 (English) 1999. CODEN: LANGD5. ISSN: 0743-7463. Publisher: American Chemical Society.

AB The characteristics of the fluorescence spectra of 2,5-bis(4-diethylaminophenyl)-1,3,4-oxadiazole (BDD) doped in **Si**-Ti binary oxides by the sol-gel method were studied as a function of time in its transitions from sol to gel to xerogel. The intensity of the fluorescence spectrum decreases with the increase in the Ti content. A characteristic BDD excimer fluorescence was obsd. during the transition from gel to xerogel only in a mixt. of tetra-Et orthosilicate (TEOS) and tetraisopropoxytitanium (TPOT) but not in pure TEOS, indicating that the presence of a **tetrahedrally** coordinated Ti ion species plays a significant role in the formation of the excimer. A possible model was proposed for the entrapment process of BDD during the sol to gel to xerogel transitions.

IT **546-68-9**, Tetraisopropoxy titanium
(fluorescence properties of 2,5-bis(4-(diethylamino)phenyl)-1,3,4-oxadiazole mols. encapsulated in SiO2 and **Si**-Ti binary oxide matrixes by sol-gel method)

RN 546-68-9 HCA

CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 22-9 (Physical Organic Chemistry)
IT Sol-gel processing
(coating; fluorescence properties of 2,5-bis(4-(diethylamino)phenyl)-1,3,4-oxadiazole mols. encapsulated in SiO_2 and **Si**-Ti binary oxide matrixes by sol-gel method)
IT Encapsulation
Excimer
Excimer fluorescence
Fluorescence
Matrix media
Xerogels
(fluorescence properties of 2,5-bis(4-(diethylamino)phenyl)-1,3,4-oxadiazole mols. encapsulated in SiO_2 and **Si**-Ti binary oxide matrixes by sol-gel method)
IT Oxides (inorganic), uses
(matrix binary; fluorescence properties of 2,5-bis(4-(diethylamino)phenyl)-1,3,4-oxadiazole mols. encapsulated in SiO_2 and **Si**-Ti binary oxide matrixes by sol-gel method)
IT Gels
(matrixes; fluorescence properties of 2,5-bis(4-(diethylamino)phenyl)-1,3,4-oxadiazole mols. encapsulated in SiO_2 and **Si**-Ti binary oxide matrixes by sol-gel method)
IT **Coating process**
(sol-gel; fluorescence properties of 2,5-bis(4-(diethylamino)phenyl)-1,3,4-oxadiazole mols. encapsulated in SiO_2 and **Si**-Ti binary oxide matrixes by sol-gel method)
IT 1679-98-7, 2,5-Bis(4-(diethylamino)phenyl)-1,3,4-oxadiazole
(fluorescence properties of 2,5-bis(4-(diethylamino)phenyl)-1,3,4-oxadiazole mols. encapsulated in SiO_2 and **Si**-Ti binary oxide matrixes by sol-gel method)
IT 78-10-4, Tetraethyl orthosilicate **546-68-9**, Tetraisopropoxy titanium
(fluorescence properties of 2,5-bis(4-(diethylamino)phenyl)-1,3,4-oxadiazole mols. encapsulated in SiO_2 and **Si**-Ti binary oxide matrixes by sol-gel method)
IT 7631-86-9, **Silicon** oxide (SiO_2), uses 13463-67-7, Titania, uses
(fluorescence properties of 2,5-bis(4-(diethylamino)phenyl)-1,3,4-

oxadiazole mols. encapsulated in SiO2 and **Si**-Ti binary oxide matrixes by sol-gel method)

L56 ANSWER 18 OF 21 HCA COPYRIGHT 2005 ACS on STN
127:294745 Organic titanosilicate-based **layered** polymers, their manufacture and moldings, and manufacture of the moldings. Tani, Masaaki; Fukushima, Yoshiaki; Okamoto, Kazuo; Yano, Kazuhisa (Toyota Central Research and Development Laboratories, Inc., Japan). Jpn. Kokai Tokkyo Koho JP 09241380 A2 19970916 Heisei, 9 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1996-83300 19960311.

AB The polymers showing UV-shielding and abrasion-resistant properties, useful for **coatings**, comprise **layered** polymers composed of (A) **tetrahedral sheets** contg. **Si** or metals as central atoms, and **octahedral sheets** contg. Ti, Mg, Al, Ni, Co, Cu, Mn, Fe, Li, V, and/or Zr as central atoms (Ti content 5-100 at.%) in which a part or all of central atoms in the tetragonal **sheets** are covalently bonding with org. groups. The polymers are manufd. by dispersing (a) organoalkoxysilanes having .gtoreq.1 alkoxy groups and .gtoreq.1 org. groups, (b) inorg. or org. salts or **alkoxides** of **Ti**, Mg, Al, Ni, Co, Cu, Mn, Fe, Li, V, and/or Zr (Ti deriv. content 5-100 at.% as Ti), and optionally, (c) **Si** alkoxide contg. .gtoreq.1 alkoxy in (d) .gtoreq.1 inorg. and/or org. polar solvents. The moldings from the above polymers are manufd. by molding the above polymers, followed by polymg. functional groups in the org. groups to link them one another. Thus, 297.6 g 3-methacryloxypropyltrimethoxysilane and 170.4 g titanium tetraisopropoxide were stirred in H2O to give 143 g powd. **layered** org. titanosilicate showing good heat resistance, dispersibility in org. solvents, and good UV shielding property.

IC ICM C08G077-02
ICS C01B033-20

CC 42-10 (Coatings, Inks, and Related Products)

ST org titanosilicate **layered** polymer sol gel; alkoxysilane inorg salt polymn ceramer prepn; heat resistance UV shield org titanosilicate

IT **Coating materials**
(heat-resistant; manuf. of org. titanosilicate-based **layered** polymers for **coatings** showing good heat resistance and UV-shielding property)

IT **Coating materials**
UV shields
(manuf. of org. titanosilicate-based **layered** polymers for **coatings** showing good heat resistance and UV-shielding property)

IT Ceramers
(manuf. of org. titanosilicate-based **layered** polymers for **coatings** showing good heat resistance and

UV-shielding property)
IT 159787-65-2P 161269-49-4P 185745-24-8P 196928-75-3P
(manuf. of org. titanosilicate-based **layered** polymers for **coatings** showing good heat resistance and UV-shielding property)

L56 ANSWER 19 OF 21 HCA COPYRIGHT 2005 ACS on STN
125:145548 Catalytic activity of Ti- and Al-pillared montmorillonite and beidellite for cumene cracking and hydrocracking. Swarnakar, R.; Brandt, Kerstin B.; Kydd, Ronald A. (Departamento de Engenharia Quimica, Universidade Federal da Paraiba, Campina Grande, P.B., Brazil). Applied Catalysis, A: General, 142(1), 61-71 (English) 1996. CODEN: ACAGE4. ISSN: 0926-860X. Publisher: Elsevier.
AB Titanium- and aluminum-pillared beidellite and montmorillonite clays were prepd. from Mg-beidellite synthesized hydrothermally, and Mg-montmorillonite obtained by Mg2+ ion exchange of a natural montmorillonite (STx-1, Source Clay Minerals Repository). The pillaring solns. were prepd. by hydrolysis of aluminum chloride and titanium tetraethoxide solns., to produce the tridecameric "Al13" polyoxocation, AlO4Al12(OH)24(H2O)127+, and "Tix" polyoxocations (structure not known), resp. X-ray diffraction anal. of the basal spacing (d001) of the samples showed that the Ti-pillared beidellite is thermally more stable than analogous montmorillonite. The order of the overall activity for cumene conversion of the clay samples is found to be: Mg-montmorillonite < Al13-montmorillonite = Tix-montmorillonite < Mg-beidellite < Tix-beidellite < Al13-beidellite. While the conversions were very different, the selectivity of beidellite based catalysts for cracking (measured by benzene produced) was consistently in the range of 86-93% and was not influenced by the presence of aluminum or titanium oxide pillars. However this was not the case for montmorillonite. Mg-STx-1 had a relatively lower benzene selectivity (36%), and both Al2O3 and TiO2 pillars increased this significantly. The difference probably arises because the beidellite surface is more acidic due to its **tetrahedral layer** charge, hence making the effect of pillars less crit.
IT **3087-36-3**, Titanium tetraethoxide
(hydroltsis of titanium tetraethoxide in prepn. of Ti-pillared montmorillonite and beidellite for cumene cracking and hydrocracking)
RN 3087-36-3 HCA
CN Ethanol, titanium(4+) salt (9CI) (CA INDEX NAME)

H_3C-CH_2-OH

●1/4 Ti(IV)

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 67

IT **3087-36-3**, Titanium tetraethoxide
(hydroltsis of titanium tetraethoxide in prepn. of Ti-pillared montmorillonite and beidellite for cumene cracking and hydrocracking)

L56 ANSWER 20 OF 21 HCA COPYRIGHT 2005 ACS on STN
122:329039 Synthesis and characterization of a (Zn, Ti)-substituted **layered** silicate. Luca, Vittorio; MacLachian, Dugald. J.; Howe, Russell F.; Bramley, R. (Res. Sch. Chem., Australian Natl. Univ., Canberra, ACT 0200, Australia). Journal of Materials Chemistry, 5(4), 557-64 (English) 1995. CODEN: JMACEP. ISSN: 0959-9428. Publisher: Royal Society of Chemistry.

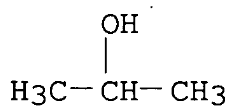
AB The incorporation of TiIV into the framework of Zn-substituted fluorohectorite is reported. Various spectroscopic techniques point to the substitution of TiIV into predominantly the **octahedral** rather than **tetrahedral** sublattice of the smectite framework. For clay particles prepd. from a reactant compn. with Ti/Ti + **Si** = 0.063 (ZTFH), energy-dispersive x-ray anal. of the particles obsd. by TEM indicates that Ti accounts for .apprx.6% of the Ti + **Si**. X-ray absorption near-edge spectra indicate that the TiIV in these clay particles is predominantly in an **octahedral** coordination. This is supported by EPR spectra of an oriented **film** sample in which TiIV is reduced to TiIII by heating the sample to 450.degree. in 30 torr of CO. The obsd. single-ion TiIII EPR spectrum shows dramatic dependence of the orientation of the clay **film** in the magnetic field. This orientation dependence is consistent with the principal g-tensor axis of the TiIII site being perpendicular to the clay **layers**. The EPR parameters of this TiIII species are consistent with TiIII occupying an **octahedral** site. Three-pulse electron spin-echo modulation data taken at the TiIII EPR line position shows modulation at the 7Li nuclear frequency and simulation indicates that TiIII ions are at 0.30-0.35 nm from LiI ions, a distance that is consistent with these two ions occupying adjacent sites in the **octahedral sheet**. The MASNMR spectrum of the Zn/Ti-substituted fluorhectorite consists of an intense Q3 resonance at -96.4 ppm and a weak shoulder at .apprx.-92.5 ppm. These two resonances are interpreted as due to

variations in the **octahedral sheet** compn.
Therefore TiIV appears to have a strong preference for occupation of the **octahedral** sites in the Zn-substituted fluorohectorite framework.

IT **546-68-9, Titanium isopropoxide**
(prepn. and **layer** structure of zinc- and titanium zinc-substituted fluorohectorite smectite clays, sodium or magnesium exchanged)

RN 546-68-9 HCA

CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 78-5 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 67

ST silicate **layered** fluorohectorite titanium zinc substituted; smectite clay fluorohectorite titanium zinc substituted

IT Clays, preparation
(smectitic, fluorohectorite; prepn. and **layer** structure of zinc- and titanium zinc-substituted fluorohectorite smectite clays, sodium or magnesium exchanged)

IT 78-10-4, Tetraethoxysilane **546-68-9, Titanium isopropoxide** 1310-73-2, Sodium hydroxide, reactions 7646-85-7, Zinc chloride, reactions 7681-49-4, Sodium fluoride, reactions 7789-24-4, Lithium fluoride, reactions
(prepn. and **layer** structure of zinc- and titanium zinc-substituted fluorohectorite smectite clays, sodium or magnesium exchanged)

L56 ANSWER 21 OF 21 HCA COPYRIGHT 2005 ACS on STN

119:232138 Preparation and characterization of aluminum titanate plasma spray powder. Shyu, L. J.; Brice, V. T.; Cambria, F. M.; Su, B. M.; Tirendi, C.; Wandass, J. (Akzo Chem. Inc., Dobbs Ferry, NY, 10522, USA). Materials Research Society Symposium Proceedings, 249(Synthesis and Processing of Ceramics: Scientific Issues), 115-20 (English) 1992. CODEN: MRSPDH. ISSN: 0272-9172.

AB Aluminum titanate ceramic powder, used in plasma spray coating as a wear resistant material, was prepd. from a gel precursor followed by high temp. calcination. The chem. derived gel was made from aluminum sulfate and **titanium isopropoxide** in an oxalic acid aq. system. The sol. complex was studied by 13C NMR

spectroscopy which showed that the mole ratio of oxalic acid bound to Al and Ti was 2:1. A copptn. took place when ammonium hydroxide was added. The gel was examd. by solid-state NMR spectroscopy which suggested that aluminum titanium hydroxyl oxalate was present with Al in a distorted **octahedral** environment. EDX mapping showed that Al and Ti were evenly distributed throughout the gel particles. Thermal anal. indicated that dehydration and combustion of org. groups took place between 100 and 400.degree.C. Gel which was heat treated at 1500.degree.C was identified as a pure Al2TiO5 cryst. phase by XRD.

CC 57-2 (Ceramics)
Section cross-reference(s): 49

IT **Coating process**
(plasma spraying, aluminum titanate powder for, sol-gel prepn. of)

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L57 ANSWER 1 OF 8 HCA COPYRIGHT 2005 ACS on STN

139:206584 Reactivity Studies, Structural Characterization, and Thermolysis of Cubic Titanosiloxanes: Precursors to Titanosilicate Materials Which Catalyze Olefin Epoxidation. Murugavel, Ramaswamy; Davis, Paul; Shete, Vivekanand S. (Department of Chemistry, Indian Institute of Technology, Mumbai, 400 076, India). Inorganic Chemistry, 42(15), 4696-4706 (English) 2003. CODEN: INOCAJ. ISSN: 0020-1669. OTHER SOURCES: CASREACT 139:206584. Publisher: American Chemical Society.

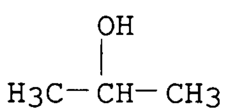
AB The cubic titanosiloxane [RSiO3Ti(OPri)]4 (R = 2,6-Pr2iC6H3NSiMe3) (1) is relatively inert in its attempted reactions with alcs. and other acidic H contg. compds. The reaction of 1 with silanol (ButO)3SiOH however proceeds over a period of .apprx.3 mo to result in the hydrolysis of (ButO)3SiOH and yield the transesterification product [RSiO3Ti(OBut)]4 (2) rather than the expected [RSiO3Ti(OSi(OBut)3)]4. Products 1 and 2 were characterized by elemental anal., thermal anal., and spectroscopic techniques (IR, EI-MS, and NMR). The solid-state structures of both 1 and 2 were detd. by single-crystal x-ray diffraction studies. Compds. 1 and 2 are isomorphous and crystallize in a cubic space group with a central cubic Ti4Si4O12 core. Solid state thermolysis of 1 was carried at 450, 600, 800, 900, 1000, and 1200.degree. in air, and the resulting titanosilicate materials were characterized by spectroscopic (IR and DR UV), powder XRD, and electron microscopic methods. While, the presence of Ti-O-**Si** linkages appears to be dominant in the samples prepd. at lower temps. (450-800.degree.), phase sepn. of anatase and rutile forms of TiO2 occurs at temps. >900.degree. as revealed by IR spectral and PXRD studies. The presence of **octahedral** Ti centers was obsd.

by diffuse reflectance UV spectroscopy for the samples heated at higher temps. The use of new titanosilicate materials as catalysts for olefin epoxidn. was studied. The titanosilicate materials produced at temps. <800.degree. with a large no. of Ti-O-**Si** linkages (or **tetrahedral** Ti centers) are more active catalysts compared to the materials produced >900.degree.. The obsd. conversion in the epoxidn. reactions is somewhat low although the selectivity of the epoxide formation over the other possible oxidized products is very good.

IT **546-68-9**, Titanium tetraisopropoxide
(reactant for prepn. of titanosiloxane deriv.)

RN 546-68-9 HCA

CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75

IT **546-68-9**, Titanium tetraisopropoxide 163631-37-6
(reactant for prepn. of titanosiloxane deriv.)

L57 ANSWER 2 OF 8 HCA COPYRIGHT 2005 ACS on STN

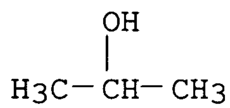
138:361645 Synthesis and structure characterization of a new Cs removal open-framework silicotitanate (Na4Ti4Si3O10). Yu, Bo; Chen, Jing; Song, Chong-Li (Institute of Nuclear Energy Technology, Tsinghua University, Beijing, 100084, Peop. Rep. China). Wuji Huaxue Xuebao, 19(2), 119-124 (Chinese) 2003. CODEN: WHUXEO. ISSN: 1001-4861. Publisher: Wuji Huaxue Xuebao Bianjibu.

AB A novel open-framework silicotitanate (Na4Ti4Si3O10) with high surface area was synthesized by a combination of sol gel-hydrothermal method. The crystal structure of Na4Ti4Si3O10 was characterized by x-ray diffraction, scanning electron microscope, and transmission electron micrograph. The compd. is tetragonal, P43, a = b 7.8110, c 11.9735 A, .alpha. = .beta. = .gamma. 90..degree.. Na4Ti4Si3O10 has a three dimensional framework constitution of Ti-O **octahedral** clusters and **Si** -O **tetrahedra**. The chem. stability, thermal stability and the Cs removal property of Na4Ti4Si3O10 were also studied.

IT **546-68-9, Titanium isopropoxide**
(for prepn. of sodium silicotitanate (Na4Ti4Si3O10))

RN 546-68-9 HCA

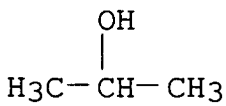
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



● 1/4 Ti(IV)

CC 78-5 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 60, 75
IT 78-10-4, Tetraethoxysilane **546-68-9, Titanium isopropoxide** 1310-73-2, Sodium hydroxide, reactions
(for prepn. of sodium silicotitanate (Na4Ti4Si3O10))

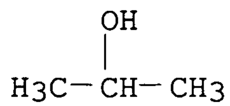
L57 ANSWER 3 OF 8 HCA COPYRIGHT 2005 ACS on STN
138:65523 Synthesis, structure characterization, and ion exchange properties of a novel open-framework ecomaterial silicotitanate. Yu, Bo; Wen, Mingfen; Chen, Jing; Song, Chongli (Institute of Nuclear Energy Technology, Tsinghua University, Beijing, 100084, Peop. Rep. China). Rare Metals (Beijing, China), 21(3), 170-174,223 (English) 2002. CODEN: RARME8. ISSN: 1001-0521. Publisher: RM Mini-Computer Publishing Office.
AB A novel open-framework ecomaterial silicotitanate (Na4Ti4Si3O10) was synthesized by a combination of sol-gel and hydrothermal methods. The study on ion exchange properties shows that Na4Ti4Si3O10 exhibits high adsorption for Cs, i.e., Kd is .ltoreq.60,000 mL/g in neutral soln. The crystal structure of Na4Ti4Si3O10 was characterized by XRD, scanning electronic microscope (SEM), transmission electron microscope (TEM), Raman spectrum, differential thermal and TGA (DTA/TGA), inductively coupled plasma (ICP), and X fluorescence anal. The compd. is tetragonal, space group P42, a 0.78110, c 1.196 45 nm, Z = 4, and Ra = 0.041; Na4Ti4Si3O10 has a three dimensional framework consisting of Ti-O **octahedral** clusters and **Si**-O **tetrahedra.** Na4Ti4Si3O10 has good chem. stability, thermal stability, and high Cs ion exchange capacity in the whole pH range.
IT **546-68-9, Titanium**(4+) **isopropoxide**
(reactant for prepn. of sodium silicotitanate)
RN 546-68-9 HCA
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 78-5 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 60, 75
IT 78-10-4, Tetraethoxysilane **546-68-9, Titanium (4+) isopropoxide** 1310-73-2, Sodium hydroxide, reactions
(reactant for prepn. of sodium silicotitanate)

L57 ANSWER 4 OF 8 HCA COPYRIGHT 2005 ACS on STN
134:62150 Pore Surface Functionalization of MCM-48 Mesoporous Silica with Tungsten and Molybdenum Metal Centers: Perspectives on Catalytic Peroxide Activation. Morey, M. S.; Bryan, J. D.; Schwarz, S.; Stucky, G. D. (Chemistry Department, University of California, Santa Barbara, CA, 93106, USA). Chemistry of Materials, 12(11), 3435-3444 (English) 2000. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.
AB The pore surface of MCM-48 mesoporous silica was functionalized with tungsten and molybdenum metal centers by the anhyd. reaction of metal alkoxides with surface silanol groups. Resulting metal-oxo species were attached via covalent M-O-**Si** bonds as confirmed with photoacoustic (PAS)-FTIR. Diffuse reflectance UV-visible spectroscopy indicates that the metal oxo groups are predominantly comprised of **tetrahedral** and **octahedral** coordinated monomers. MCM-48 grafted with Mo and W is active for brominating phenol red with hydrogen peroxide at neutral pH in a manner similar to Ti-MCM-48, as we reported earlier. The rates of bromination for Mo, W, and four other metals, after normalization for metal concn., measured as absorption peak intensities of the resultant bromophenol blue, are as follows: 50p46:16:2.8p1:0 W:Mo:Ti:Zr:V:Re. The different rates of reactivity, and hence the general degree of metal-peroxo activation, can be explained on the basis of size, charge, coordination sphere, and electronegativity of the central metal.
IT **546-68-9**, Titanium tetraisopropoxide
(pore surface functionalization of MCM-48 mesoporous silica with tungsten and molybdenum metal centers and perspectives on catalytic peroxide activation)
RN 546-68-9 HCA
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 22, 66

IT **546-68-9**, Titanium tetraisopropoxide 5588-84-1, Triisopropoxyvanadium oxide 7722-84-1, Hydrogen peroxide, reactions 23519-77-9, Zirconium tetrapropoxide 26143-11-3, Tungsten pentaethoxide 74060-96-1
(pore surface functionalization of MCM-48 mesoporous silica with tungsten and molybdenum metal centers and perspectives on catalytic peroxide activation)

L57 ANSWER 5 OF 8 HCA COPYRIGHT 2005 ACS on STN

132:323257 Synthesis, characterization and photocatalytic properties of titania-modified mesoporous silicate MCM-41. Zheng, Shan; Gao, Lian; Zhang, Qing-hong; Guo, Jing-kun (Shanghai Institute of Ceramics, State Key Lab of High Performance Ceramics and Superfine Microstructure, Chinese Academy of Sciences, Shanghai, 200050, Peop. Rep. China). Journal of Materials Chemistry, 10(3), 723-727 (English) 2000. CODEN: JMACEP. ISSN: 0959-9428. Publisher: Royal Society of Chemistry.

AB A series of titania modified mesoporous silicate MCM-41 (MCM-TiO2) samples with variable Ti/**Si** ratio were prepd. from tetra-Bu titanate and calcined MCM-41. The samples were characterized by powder x-ray diffraction, FTIR spectroscopy, thermal anal. (DTA-TG), nitrogen adsorption-desorption at 77 K, TEM, and solid state diffuse reflectance UV-VIS spectroscopy. Tetra-Bu titanate co-condensation on OH groups of MCM-41 led to **Si** -O-Ti bonds, modifying the inner pore surface of MCM-41 after hydrolysis and calcination. The titania modified MCM-41, titania species show **tetrahedral** rather than **octahedral** coordination which is predominant in cryst. titania, and exhibit good photocatalytic activity in photoinduced oxidn. of phenol in aq. soln. to carbon dioxide and water. The photocatalytic system is of interest for decompn. of phenol and other org. compds. in environmental samples.

IT **5593-70-4**, Tetrabutyl titanate
(prepn. and catalytic activity of titania-modified mesoporous zeolite MCM-41 in photooxidn. of phenol towards treatment of contaminated environmental media)

RN 5593-70-4 HCA
CN 1-Butanol, titanium(4+) salt (9CI) (CA INDEX NAME)

$H_3C-CH_2-CH_2-CH_2-OH$

●1/4 Ti(IV)

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 59, 61, 67
IT **5593-70-4**, Tetrabutyl titanate
(prepn. and catalytic activity of titania-modified mesoporous zeolite MCM-41 in photooxidn. of phenol towards treatment of contaminated environmental media)

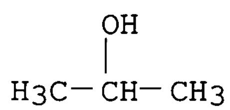
L57 ANSWER 6 OF 8 HCA
132:302377 Hydrothermal and Postsynthesis Surface Modification of Cubic, MCM-48, and Ultralarge Pore SBA-15 Mesoporous Silica with Titanium. Morey, Mark S.; O'Brien, Stephen; Schwarz, Stephan; Stucky, Galen D. (Department of Chemistry and Materials Research Laboratory, University of California, Santa Barbara, CA, 93106, USA). Chemistry of Materials, 12(4), 898-911 (English) 2000. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.
AB The authors describe the introduction of titanium centers to cubic MCM-48 and SBA-15 mesoporous silica by hydrothermal and postsynthetic grafting techniques. MCM-48 was hydrothermally prepd. with a gemini surfactant that favors the cubic phase and leads to a high degree of long-range pore ordering. This phase was chosen due to its high surface area (1100-1300 m2/g) and its three-dimensional, bicontinuous pore array. SBA-15, synthesized with a block copolymer template under acidic conditions, has a surface area from 600 to 900 m2/g and an av. pore diam. of 69 .ANG., compared to 24-27 .ANG. for MCM-48. **Alkoxide** precursors of **titanium** were used to prep. samples of Ti-MCM-48 and Ti-SBA-15. The authors have detailed the bulk and mol. structure of both the silica framework and the local bonding environment of the titanium ions within each matrix. X-ray powder diffraction and nitrogen adsorption shows the pore structure is maintained despite some shrinkage of the pore diam. at high Ti loadings by grafting methods. UV-visible and Raman spectroscopy indicate that grafting produces the least amt. of Ti-O-Ti bonds and instead favors isolated **tetrahedral** and **octahedral** titanium centers. High-resoln. photoacoustic FTIR spectra demonstrated the presence of intermediate range order within the silicate walls of MCM-48, established the consumption of surface silanols to form **Si**-O-Ti bonds by grafting, and resolved the characteristic IR absorbance at 960 cm-1, occurring in

titanium silicates, into two components. All three spectroscopic techniques, including in situ Raman, reveal the reactive intermediates formed when the materials are contacted with hydrogen peroxide.

IT **546-68-9, Titanium isopropoxide**
(reactant for prepn. of Ti surface grafted MCM-48 and SBA-15)

RN 546-68-9 HCA

CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 78-4 (Inorganic Chemicals and Reactions)

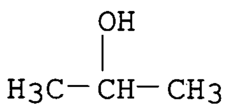
IT **546-68-9, Titanium isopropoxide**
(reactant for prepn. of Ti surface grafted MCM-48 and SBA-15)

L57 ANSWER 7 OF 8 HCA COPYRIGHT 2005 ACS on STN

128:187796 Synthesis and crystal structure of Na4[(TiO)4(SiO4)3].cntdot.6H2O, a rhombohedrally distorted sodium titanium silicate pharmacosiderite analog. Dadachov, Mike S.; Harrison, William T. A. (Materials Division, Australian Nuclear Science and Technology Organisation, New South Wales, 2234, Australia). Journal of Solid State Chemistry, 134(2), 409-415 (English) 1997. CODEN: JSSCBI. ISSN: 0022-4596. Publisher: Academic Press.

AB The synthesis and crystal structure of Na4[(TiO)4(SiO4)3].cntdot.6H2O, a new hydrated Na Ti silicate with the rhombohedrally distorted pharmacosiderite structure type, are reported. Na4[(TiO)4(SiO4)3].cntdot.6H2O was synthesized as a powder by the low temp. hydrothermal crystn. of an alk. Ti silicate gel prepd. via a novel peroxide route. Its structure was detd. and refined by the Rietveld method using x-ray powder data. The three-dimensional framework of Na4[(TiO)4(SiO4)3].cntdot.6H2O is built up from clusters of four edge-sharing TiO6 **octahedra,** connected by **tetrahedrally** coordinated **Si** atoms (isolated SiO4 groups). The large extra-framework cages contain H2O mols. and are linked to each other via eight-membered rings (.apprx. 5 .ANG. in diam.). Two distinct Na cations are located: one in the off-center position of the eight-membered ring and another in the internal corner of cage. Crystal data: Na4[(TiO)4(SiO4)3].cntdot.H2O, Mr = 719.8, rhombohedral, space group R3m, a 7.8124(6) .ANG., .alpha. 88.794(9), Z = 1, Rp = 0.09, Rwp = 0.12.

IT 546-68-9, Titanium tetraisopropoxide
(for prepn. of sodium titanium silicate
Na4[(TiO)4(SiO4)3].cntdot.6H2O)
RN 546-68-9 HCA
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)



●1/4 Ti(IV)

CC 78-4 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75
IT **546-68-9**, Titanium tetraisopropoxide 1310-73-2, Sodium hydroxide (NaOH), reactions 7440-21-3, **Silicon**, reactions 7722-84-1, Hydrogen peroxide (H2O2), reactions 13780-39-7, Titanium chloride oxide (TiCl2O)
(for prepn. of sodium titanium silicate
Na4[(TiO)4(SiO4)3].cntdot.6H2O)

L57 ANSWER 8 OF 8 HCA COPYRIGHT 2005 ACS on STN
128:175268 Electron Spin Resonance Evidence for Isomorphous Substitution of Titanium into Titanosilicate TiMCM-41 Mesoporous Molecular Sieve. Prakash, A. M.; Sung-Suh, Hyung Mi; Kevan, Larry (Department of Chemistry, University of Houston, Houston, TX, 77204, USA). Journal of Physical Chemistry B, 102(5), 857-864 (English) 1998. CODEN: JPCBFK. ISSN: 1089-5647. Publisher: American Chemical Society.
AB New evidence for the framework substitution of titanium into TiMCM-41 mesoporous mol. sieve is found from ESR studies. TiMCM-41 samples with varying **Si**/Ti ratios were synthesized as have titanosilicate TS-1, siliceous MCM-41, AlMCM-41, and Ti-AlMCM-41 in the last of which titanium ions are incorporated by ion exchange. These materials were examd. by ESR spectroscopy after a thermal activation treatment followed by .gamma.-irradn. at 77 K. .gamma.-Irradn. at 77 K of TiMCM-41 having a high **Si**/Ti ratio produces a strong orthorhombic ESR signal due to V centers and an axial signal with g.dblvert. = 1.971 and g.perp. = 1.901 best explained as arising from trivalent titanium situated at a framework **tetrahedral** site. An upper limit for the substitution of titanium into a framework **tetrahedral** site is obsd. As the titanium concn. in the synthesis gel increases, the resulting material contains both **tetrahedral** and **octahedral** titanium. .gamma.-Irradn. of ion-exchanged Ti-AlMCM-41 gives an axial ESR signal characterized by reverse g values g.dblvert. =

1.898 and g:perp. = 1.967 typical of Ti(III) in distorted **octahedral** symmetry. Both TiMCM-41 and Ti-AlMCM-41 differ in their behavior toward interaction with various adsorbate mols. The Ti(III) species obsd. in TiMCM-41 after adsorption of D2O, CO, NH3, and CD3OH changes its ESR characteristics from that of the original Ti(III) species obsd. in the absence of these adsorbates. The ESR characteristics of the Ti(III) species in Ti-AlMCM-41 after adsorption of the above adsorbates are different from those of TiMCM-41, indicating that the Ti in these two materials are in different coordination environments. This independently supports the different g tensors for Ti(III) in TiMCM-41 vs. Ti-AlMCM-41.

IT **3087-36-3, Titanium**(IV) **ethoxide**
(for prepn. of titanosilicate TiMCM-41)

RN 3087-36-3 HCA

CN Ethanol, titanium(4+) salt (9CI) (CA INDEX NAME)

H_3C-CH_2-OH

● 1/4 Ti(IV)

CC 78-4 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 77

IT 1344-09-8, Sodium silicate **3087-36-3, Titanium** (IV) **ethoxide**
(for prepn. of titanosilicate TiMCM-41)